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1998 J. Phys.: Condens. Matter 10 2993

(http://iopscience.iop.org/0953-8984/10/13/016)

J. Phys.: Condens. Matter **10** (1998) 2993–3001. Printed in the UK PII: S0953-8984(98)86942-7

Bistability of resonant electron tunnelling through degenerate states of a quantum well

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Received 12 August 1997, in final form 18 November 1997

Abstract. Within the approach of low-transparency barriers, the tunnelling of electrons through a double-barrier system taking into account their Coulomb interaction in the interbarrier space (a quantum well) has been considered. The state of the electrons in the quantum well is supposed to be N-fold degenerate. It was shown that the dependence of the tunnelling current on the applied voltage has a steplike form at low temperatures and has a threshold in the region of small applied voltages. The system considered also exhibits bistability properties.

1. Introduction

Resonant electron tunnelling of particles through a system of double potential barriers is very sensitive to the position of electronic states in a quantum well [1–3]. This circumstance can be used for effective governing of the tunnelling process. For example, it is possible to change the potential field in the well by accumulation of electric charge in the system under tunnelling [4]. This process supposes the existence of a large number of electronic states in the interbarrier space. Actually such a condition requires that the system has a macroscopic size for which a concept of electric capacitance can be introduced [5]. In the case of a small-area quantum well one should consider electron–electron interaction using the quantum mechanical description with account of its influence on the tunnelling. For electrons that are tunnelling through a quantum dot, this problem has been considered in reference [6]. In particular, it was shown that the conductance oscillations are approximately periodic only for a large number of electrons. It was predicted that for a small number of electrons a 'shell' structure can be observed in the oscillations. The case with a small number of electrons is the most interesting one. As will be shown below, the influence of Coulomb interaction on the tunnelling process substantially increases when the states in the quantum well become degenerate. We shall consider this problem for the case of an N-fold-degenerate electronic state, in which the accumulation of up to N electrons is possible. We confine our analysis to detailed consideration of the cases of doubly and triply degenerate states. The inclusion of interaction between electrons can lead to some regularities typical of nonlinear tunnelling, e.g. to a steplike form of the current–voltage characteristics, and to tunnelling bistability. Study of fluctuations in these systems shows that they can be virtually suppressed. This is typical of double-level systems [7].

2. The Hamiltonian of the system

As the model of the double-barrier tunnelling system, we will consider a structure with the energy profile shown in figure 1. The Hamiltonian describing the tunnelling of electrons

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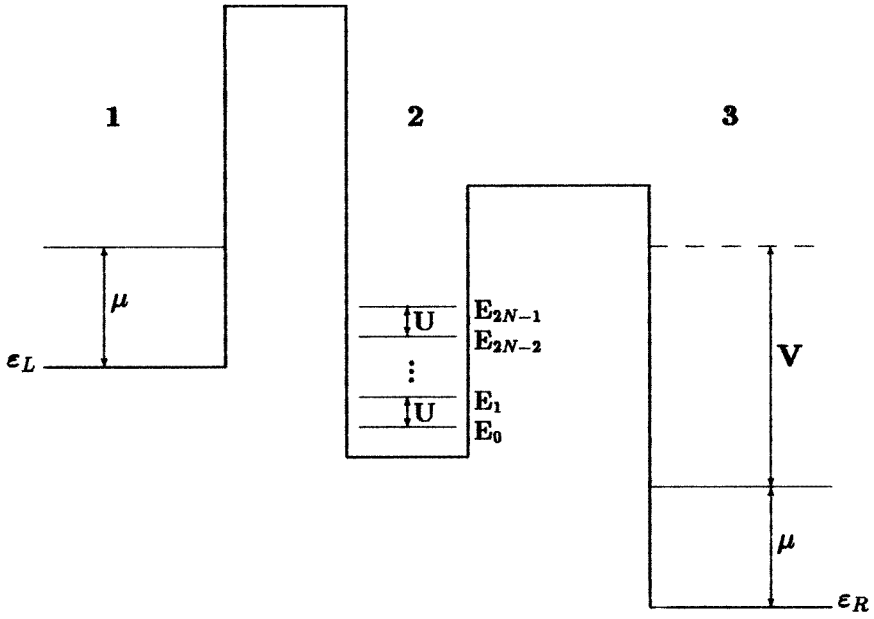

Figure 1. The energy profile of a double-barrier system with the applied voltage V.

through such a structure can be chosen to have the form

$$H = H_0 + H_W + H_T. \tag{1}$$

The first term of this Hamiltonian

$$H_0 = \sum_{k\sigma} \varepsilon_L(k) a^+_{k\sigma} a_{k\sigma} + \sum_{p\sigma} \varepsilon_R(p) a^+_{p\sigma} a_{p\sigma} \tag{2}$$

describes electrons in the left-hand electrode–emitter (the first term) and in the right-hand electrode–collector (the second term), respectively (regions 1 and 3 in figure 1). Here $a^+_{k\sigma}$ $(a_{k\sigma})$ and $a^+_{p\sigma}$ $(a_{p\sigma})$ are the creation (annihilation) operators for the electrons in the emitter and the collector, respectively, $\varepsilon_L(k) = \varepsilon_L + \hbar^2 k^2/2m_L$ is the energy of electrons in the emitter, $\hbar k$ and m_L are their quasimomentum and effective mass, respectively, and σ is the electron spin. For the collector, with an external potential V applied across the system taken into account, we have $\varepsilon_R(p) = \hbar^2 p^2/2m_R + \varepsilon_R - V$, $\hbar p$ being the quasimomentum and m_R the effective mass. The Hamiltonian H_W describes the electronic states in the quantum well (region 2 in figure 1). We consider the case in which the quantum well has an N-fold-degenerate state. In this case, H_W can be written in the form

$$H_W = \sum_{\alpha} E_0 a^+_{\alpha} a_{\alpha} + \frac{1}{2} \sum_{\alpha_1 \alpha_2} V_{\alpha_1 \alpha_2} a^+_{\alpha_1} a^+_{\alpha_2} a_{\alpha_2} a_{\alpha_1} \tag{3}$$

where $\alpha = (l, \sigma)$, σ is the spin number, and l is the number of the quantum state, taking values from 1 to N. The energy of the degenerate state in the well, with account taken of the applied voltage, is written as follows: $E_0 = \varepsilon_0 - \gamma V$, where ε_0 is the energy of the resonant state in the quantum well, and γ is a factor depending on the profile of the potential barriers (for identical barriers, $\gamma = 0.5$), and V_{α_1,α_2} is a matrix element for the electron–electron interaction in the interbarrier space. For simplicity, we approximate this

element by a positive constant $V_{\alpha_1,\alpha_2} = U$ corresponding to repulsion. The Hamiltonian H_T describing the tunnelling of electrons through the barriers has the conventional form [8]

$$H_T = \sum_{k\alpha} T_{k\alpha} a^+_{k\sigma} a_\alpha + \sum_{\alpha p} T_{p\alpha} a^+_{p\sigma} a_\alpha + \text{c.c.} \tag{4}$$

where $T_{k\alpha}$ and $T_{p\alpha}$ are the matrix elements for tunnelling through the emitter and the collector, respectively. In the general case, they depend on the applied voltage.

3. The density of states

The density of states $\rho(E)$ in the quantum well can be defined by using the retarded Green's function $G(\alpha, \alpha, E)$:

$$\rho(E) = -\frac{1}{\pi} \sum_{\alpha} \operatorname{Im} G(\alpha, \alpha, E) \tag{5}$$

where $G(\alpha, \alpha, E)$ is the Fourier transform of the retarded Green's function:

$$G(\alpha, \alpha, t) = -\mathrm{i}\theta(t) \langle [a^+_\alpha(t), a_\alpha(0)]_+ \rangle \tag{6}$$

and $\theta(t)$ is the unit Heaviside function. Using the Hamiltonian H_W, the Green's function can be calculated exactly. So for the state of quantum number α, one can obtain

$$G(\alpha, \alpha, E) = \frac{1}{(E' - E_0)} \left\{ 1 + \sum_{m=1}^{2N-1} \sum_{\substack{\alpha_1,\ldots,\alpha_m \neq \alpha \\ \alpha_1 \neq \alpha_2 \neq \cdots \neq \alpha_m}} \prod_{m_1=1}^{m} n_{\alpha_{m_1}} \frac{U}{E' - E_0 - m_1 U} \right\} \tag{7}$$

with $E' = E + \mathrm{i}\eta$ for $\eta \to +0$. Here $n_\alpha = \langle a^+_\alpha a_\alpha \rangle$ are the mean values of the occupation numbers of the state α. The Green's function has poles at $E_m = E_0 + mU$, where $m = 0, 1, 2, \ldots, 2N-1$. Thus, the electron–electron interaction leads to the splitting of the states in the quantum well. New states are separated by the gap U. Using equation (7), we can calculate the density of states in the interbarrier space. It depends on the occupation numbers n_α which are functions of the applied voltage, and hence depend on its value. This is the reason behind the nonlinearity of the tunnelling.

4. Occupation numbers for quantum states in the well

If we apply a constant external voltage to the system, a nonequilibrium steady-state distribution of electrons sets in. We assume that the electron distribution functions in the electrodes are at equilibrium by virtue of their large volumes, but that their chemical potentials change. The latter are connected through the relation $\mu_L - \mu_R = V$ (where μ_L and μ_R are the chemical potentials of the emitter and the collector, respectively). The electron distribution function $g(E)$ in the quantum well is essentially nonequilibrium. It can be determined from the condition of equality of the tunnelling current through the emitter and the collector [8, 9], and has the form

$$g(E) = \frac{1}{\Gamma(E)} [\Gamma_L(E) f_L(E) + \Gamma_R(E) f_R(E)] \tag{8}$$

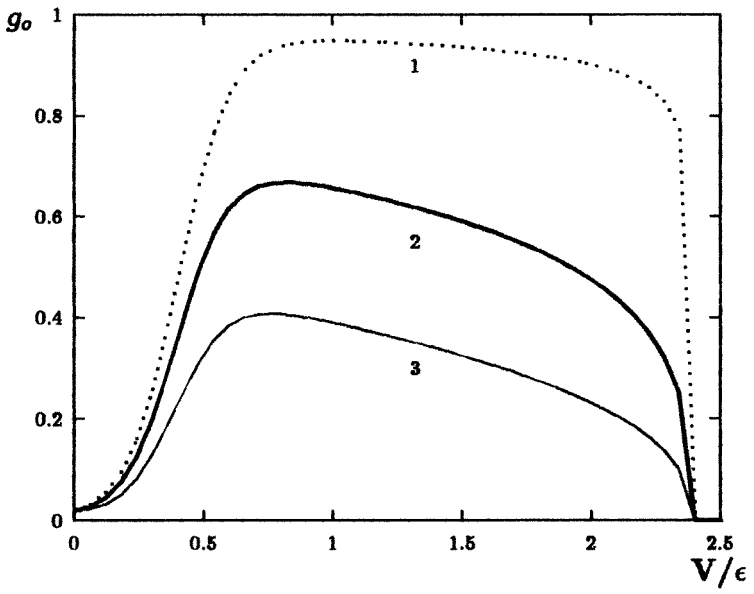

Figure 2. The dependence of the electron energy distribution function g_0 in the quantum well on the applied voltage V for various values of the ratio α_L/α_R: 30 (curve 1); 3 (curve 2); 1 (curve 3).

where

$$\begin{aligned}\Gamma(E) &= \Gamma_L(E) + \Gamma_R(E)\\ \Gamma_L(E) &= \sum_k |T_{k\alpha}|^2 \delta[E - \varepsilon_L(k)]\\ \Gamma_R(E) &= \sum_p |T_{p\alpha}|^2 \delta[E - \varepsilon_R(p)].\end{aligned} \tag{9}$$

$f_L(E)$ and $f_R(E)$ are electron distribution functions in the emitter and the collector, respectively. The occupancy of the states in the quantum well can be determined with the help of the expression [10]

$$n_\alpha = -\frac{1}{\pi}\int \mathrm{d}E\ g(E)\,\mathrm{Im}\,G(\alpha,\alpha,E). \tag{10}$$

As follows from (7), the expression for n_α does not depend on the index α. Therefore, the mean values of the occupation numbers are also independent of the number of the quantum state, and we can assume that $n_\alpha = n$. Thus, we finally obtain

$$n = F(n) \tag{11}$$

where

$$F(n) = \sum_{m=0}^{2N-1} C_{2N-1}^m g_m (1-n)^{2N-1-m} n^m \qquad C_{2N-1}^m = \frac{(2N-1)!}{m!(2N-1-m)!}.$$

The functions $g_m = g(E_m)$ determine the occupancy of the new states. Thus we have obtained the algorithmic equation of power $2N-1$ for the occupation numbers n. In the general case, this equation can have several solutions in the interval $0 \leqslant n \leqslant 1$. According to equation (11), when $g_m = g$ we get $n = g$.

In the one-dimensional case, in which the matrix elements of the tunnelling are independent of the momentum, the functions $\Gamma_L(E)$ and $\Gamma_R(E)$ can be approximated by the value [11]

$$\Gamma_{L,R} = \alpha_{L,R}\sqrt{E - \varepsilon_{L,R}(0)}. \tag{12}$$

Here α_L and α_R are the proportionality factors for the emitter and the collector, respectively. Substituting (12) into (8) and taking into account that

$$f_{L,R} = \left[\exp\left(\frac{E - \mu_{L,R}}{k_B T}\right) + 1\right]^{-1} \tag{13}$$

where k_B is Boltzmann constant and T is the temperature, we obtain an expression for the electron distribution function g_m. The dependence of g_0 on the applied voltage for various values of the ratio α_L/α_R and $k_B T/\epsilon = 0.001$ is shown in figure 2. ϵ is a normalizing constant having the order of magnitude μ. The functions g_m have the same form, but are displaced by mU on the energy scale.

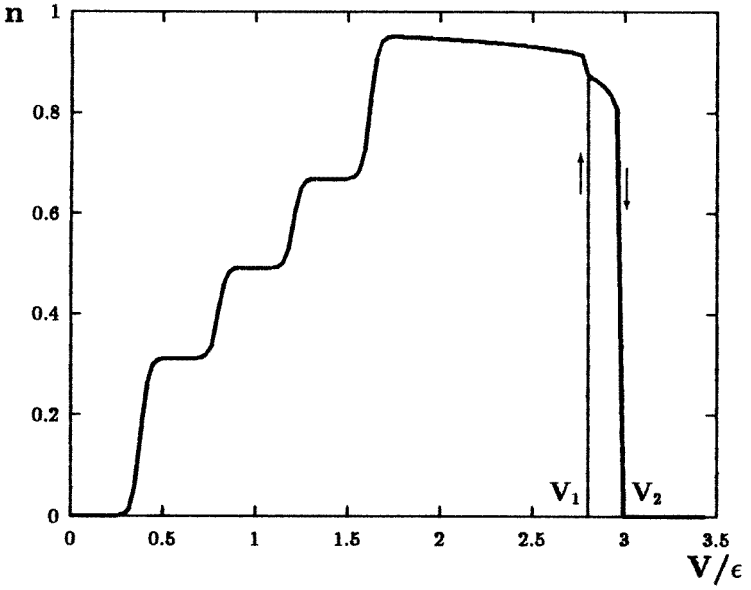

Figure 3. The dependence of the population density n of the quantum well on the applied voltage V for $k_B T/\epsilon = 0.01$ in the case where $N = 2$.

For more detailed consideration of the properties of equation (11), we will consider particular cases.

4.1. The doubly degenerate state ($N = 2$)

In this case, an analysis of equation (11) shows that in the interval $0 < n < 1$ it has three solutions for $g_0 = g_1 = 0$, i.e., when two lower states are vacant. These solutions have the form

$$n_1 = 0$$
$$n_{2,3} = -\frac{3}{2}\frac{g_2}{g_3 - 3g_2} \pm \sqrt{\frac{9g_2^2 + 4(g_3 - 3g_2)}{4(g_3 - 3g_2)^2}}. \tag{14}$$

On imposing the condition $0 < n < 1$, expression (14) leads to

$$\begin{aligned} &0 < \frac{3g_2}{3g_2 - g_3} < 2 \\ &9g_2^2 - 4(3g_2 - g_3) > 0. \end{aligned} \tag{15}$$

These inequalities, equations (15), are compatible when

$$g_2 \geqslant \frac{2}{3}(1 + \sqrt{1 - g_3}) \qquad g_3 > 3/4. \tag{16}$$

Thus, equation (11) has three solutions when the values of g_1 and g_3 are close to unity. The two solutions n_1 and n_3 are stable, while the third solution n_2 is unstable. The stable states correspond to the cases in which the well either does not contain electrons or contains four electrons occupying two upper levels. The latter is possible since the system is essentially nonequilibrium. A plot of the dependence of the occupancy n on the applied voltage at low temperature ($k_BT/\epsilon = 0.01$), and for the parameters $\alpha_L/\alpha_R = 33.3$, $\gamma = 0.5$, $\varepsilon_0/\epsilon = 1.2$, $U = 0.2/\epsilon$, obtained by solving equation (11), is represented in figure 3. It can be seen that as the applied voltage increases, the occupancy of the quantum well increases stepwise due to sequential occupation of split states. After the attainment of a certain critical value V_2, the occupation drops abruptly to zero due to the departure of the states in the quantum well from resonance. With decreasing voltage (from the value attained before), a jump of the occupancy will be observed at a lower value of the voltage V_1. Thus, the voltage range from V_1 to V_2 contains a bistability region, which is connected to the removal of electrons from the lower levels and to their attachment to the upper split states.

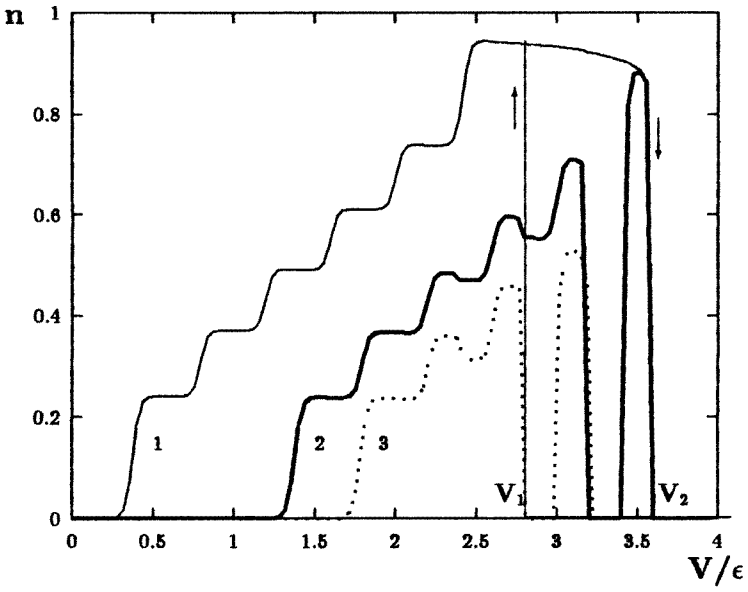

Figure 4. The dependence of the population density n of the quantum well on the applied voltage V in the case where $N = 3$ for various values of the chemical potential μ/ϵ: 1.0 (curve 1); 0.5 (curve 2); 0.3 (curve 3).

4.2. The triply degenerate state (N=3)

In the case of the triply degenerate state in the quantum well, the dependence of the occupancy n on the applied voltage is more complicated. This dependence is shown in figure 4 for the same values of the parameters as in figure 3. In this case equation (11) has a solution with the bistability state of the tunnelling at lower concentrations of charge carriers (see curves 2 and 3 in figure 4 for $\mu/\epsilon = 0.5$ and 0.3). In the case where $\mu < U$, only one term will remain in the expression for $F(n)$. Equation (11) has several solutions in the range $0 \leqslant n \leqslant 1$ when the function $B(n) = F(n)/n$ satisfies the condition $\max B(n) > 1$. For example, let only one term with energy E_2 be unequal to zero in $F(n)$. Then equation (11) takes on the form

$$n = 10g_2(1-n)^3n^2. \tag{17}$$

This equation has three solutions when $g_2 > 0.948$. Using the dependence of $E_2 = \varepsilon_0 - \gamma V + 2U$ on the applied voltage, we can find the interval of voltages over which the process of tunnelling is bistable:

$$\frac{\varepsilon_0 + 2U - \mu}{\gamma} < V < \frac{\varepsilon_0 + 2U}{\gamma}. \tag{18}$$

The dependence of n on V for $\mu/\epsilon = 0.15$ and $\alpha_L/\alpha_R = 333.3$ is shown in figure 5. It can be seen in figure 5 that steps are transformed to hollows, but the bistability is conserved. The region of bistability occupies the interval $2.9 < V < 3.2$, which agrees with inequality (18). For this range of voltages, the well can be occupied by three electrons or be empty. It is worth mentioning that the state with the energy E_2 is the only state for which the process of tunnelling may be bistable for $U < \mu$ in the case where $N = 3$. In this case, the bistability range (the right-hand peak in figure 5) does not overlap with the interval of voltages for which the tunnelling process is one valued.

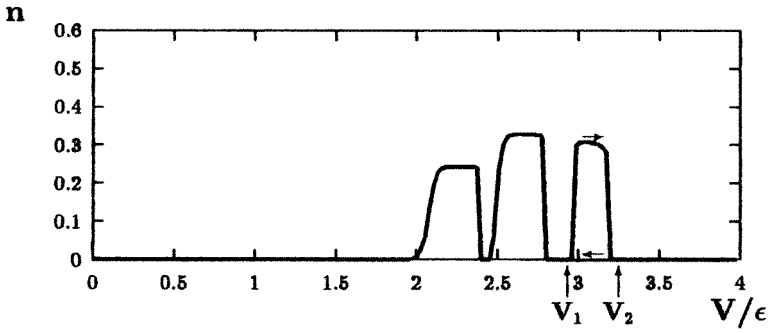

Figure 5. The dependence of the population density n of the quantum well on the applied voltage V in the case where $N = 3$ for the chemical potential $\mu/\epsilon = 0.15$, $U/\epsilon = 0.2$, and the ratio $a_L/a_R = 333.3$.

5. The tunnelling current

In the case of a constant applied voltage, the tunnelling current through the double-barrier structure can be calculated in various ways (see, for example, references [9, 11]). The

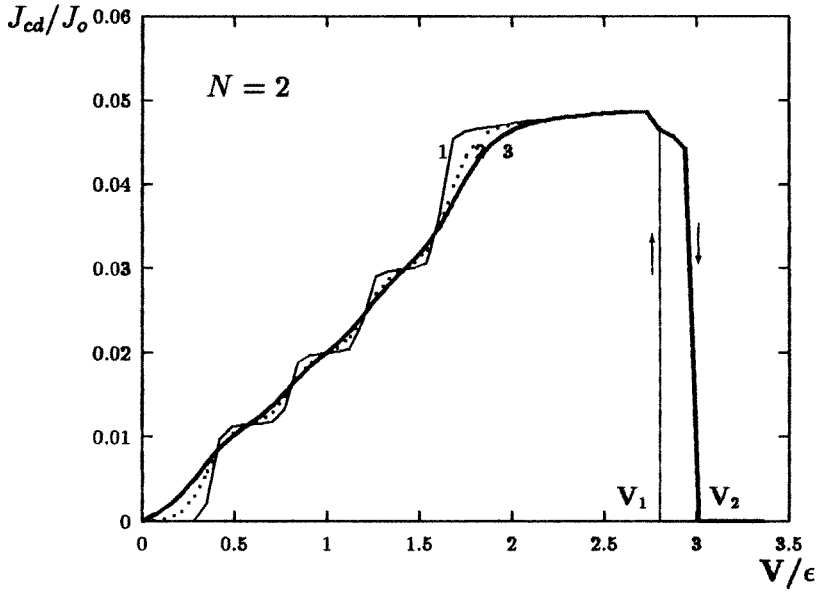

Figure 6. The dependence of the tunnelling current I_{cd}/I_0 ($I_0 = e/\bar{h}$) on the applied voltage V for various temperatures kT/ϵ: 0.01 (curve 1); 0.03 (curve 2); 0.05 (curve 3).

following simple expression was obtained for this quantity:

$$J_{cd} = \frac{e}{\bar{h}} \int \mathrm{d}E \; \frac{\Gamma_L(E)\Gamma_R(E)}{\Gamma(E)} [f_L(E) - f_R(E)]\rho(E) \tag{19}$$

where e is the electronic charge. For a low barrier transparency, $\Gamma \ll U$, the density of states can be calculated by using formulae (5) and (7):

$$\rho(E) = 4 \sum_{m=0}^{2N-1} C_{2N-m}^{m} \delta(E - E_m). \tag{20}$$

Then, the formula (19) can be transformed to

$$J_{cd} = \frac{e}{\bar{h}} \sum_{m=0}^{2N-1} \frac{\Gamma_R(E_m)\Gamma_L(E_m)}{\Gamma(E_m)} \{f_L(E_m) - f_R(E_m)\}(1-n)^{2N-1-m} n^m C_{2N-1}^{m}. \tag{21}$$

We have restricted ourselves to the case of the passage of the tunnelling current through the doubly degenerate state of the quantum well ($N = 2$). The results of numerical calculations of $J_{cd}(V)$ for the same parameters as were used for constructing the curves in figure 3 are illustrated in figure 6, for different values of the temperature. The steplike form of the dependence of the current on the applied voltage is due to the splitting of the degenerate levels. A bistability region observed at high voltage is due to the attachment of electrons to the upper energy levels.

6. Conclusion

Thus, the interaction between the electrons in a quantum well having a degenerate state results in conductance oscillations of the tunnelling system with a period proportional to the value of the Coulomb interaction U. The latter is connected to the splitting of a

degenerate electronic state by the Coulomb interaction. The steplike form of the current–voltage characteristic and the nature of its threshold resemble what one would expect for single-electron tunnelling [11] to a certain extent. The resemblance becomes even stronger if we model the quantum well by a sphere of radius b and the matrix element U of the interaction by the averaged Coulomb potential:

$$U = \frac{3}{2}\frac{e^2}{\epsilon_0 b}. \tag{22}$$

Here ϵ_0 is the dielectric permittivity of the sphere. If we use the classical definition $C = \epsilon_0 b$ of the electric capacitance of a sphere, expression (22) can be written in the form

$$U = \frac{3}{2}\frac{e^2}{C}. \tag{23}$$

This expression, which determines the magnitude of the current step, is well known in the theory of single-electron tunnelling. In our approach, however, C is interpreted as the capacitance of the well rather than the total capacitance at the barriers.

An important feature of the model under consideration is its stability against fluctuation. Indeed, a simple analysis of the fluctuations of the occupancies of the state of the well leads to

$$\langle \delta n^2 \rangle = \langle (\hat{n} - n)^2 \rangle = n(1 - n). \tag{24}$$

For the region of bistability, n assumes values close to unity or zero. For these values, $\sqrt{\langle \delta n^2 \rangle} \ll n$. However, in the region of current steps, the fluctuations are comparable with the charge. This conclusion is confirmed experimentally [12]. As the temperature increases, the steps are blurred rapidly due to the blurring of the Fermi level. The region of their existence is limited by the condition $kT \ll U$. The temperature dependence of the bistability is associated with variations of the functions g_m. The latter are less sensitive to temperature. Bistability disappears when $\max g(E) < 3/4$. This condition is satisfied even at high temperatures comparable with μ. For this temperature range, the dependence on spin can be neglected and the situation becomes similar to that analysed in reference [2].

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